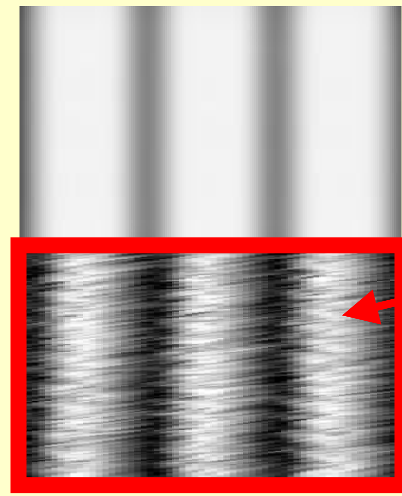
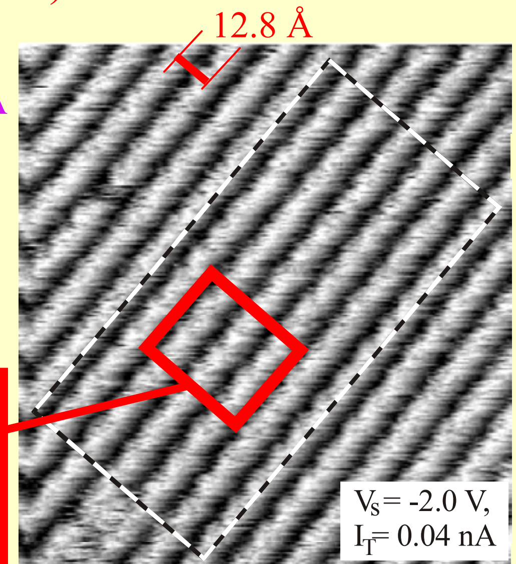
NIRT: Building Nanospintronic and Nanomagnetic Structures: Growth, Manipulation, and Characterization at the Atomic Scale

Arthur R. Smith, Saw-Wai Hla, Nancy Sandler, and Sergio E. Ulloa
Ohio University, Athens, OH, DMR-0304314
(work also partly supported by DMR-9983816).

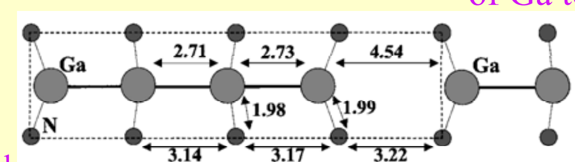
A necessary step to study magnetic phenomena on the surface of semiconductor materials, consists in obtaining a detailed understanding of surface structures. The figures at right show STM images of Ga atoms on top of GaN. In this surface reconstruction, Ga atoms arrange in groups of four, forming ordered tetramer structures lining up in rows along the [110] direction. Although dimers are common semiconductor surface units, linear Ga tetramers are quite unusual. Using the first principles method SIESTA, we also calculated the charge distribution for this particular surface reconstruction.

Simulated image of Ga Tetramers using SIESTA

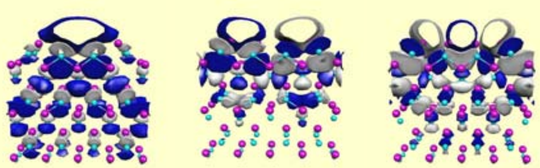




Experimental STM images of Ga tetramer rows.



Predicted tetramer unit: interatomic distances are in Angstroms.



Upper plots: occupied surface states. Amplitude is larger at the center of the tetramer where the charge is located.

Lower plots: empty surface states. The amplitudes have minima at the center of the tetramer with maxima at the dangling bonds.

Besides reproducing the STM images, we obtained detailed structural (i.e. inter-atomic distances and bond angles), and electronic structure information (i.e. surface states and band-gaps). Figures at left show wave-function amplitude for new surface states.

NIRT: Building Nanospintronic and Nanomagnetic Structures: Growth, Manipulation, and Characterization at the Atomic Scale; Arthur R. Smith, Saw-Wai Hla, Nancy Sandler, and Sergio Ulloa, Ohio University, Athens, OH, DMR-0304314. An important step in this NIRT project is studying the surface structure of nitride materials. Here we have investigated the GaN(001) 4x1 reconstruction using molecular beam epitaxy to grow the layer and then scanning tunneling microscopy to analyze the surface of the layer. Quite successfully, we have imaged the linear Ga tetramer reconstruction in real space by STM, as shown here. The significance of this direct observation is that such linear tetramers are not known to occur on other III-V (001) semiconductor surfaces, in other structures are more common such as dimers. The tetramer structure was first proposed by Neugebauer (one of our collaborators) *et al.* [*Phys Rev Lett.* ***80****, 3097(1998)*] for this surface. Before our work, the 4x1 reconstruction has been measured using reflection high energy electron diffraction (a reciprocal space technique). This work has been submitted for publication.

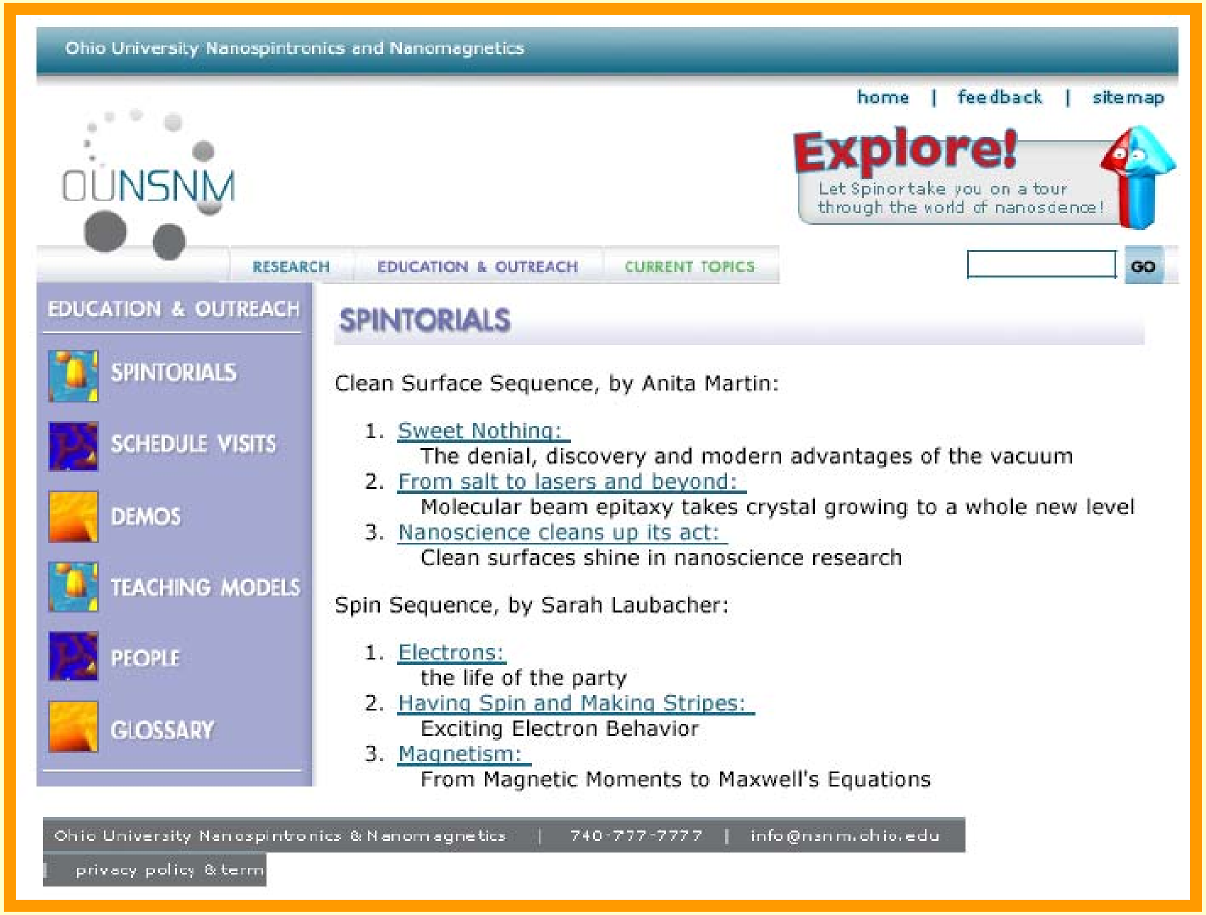
Besides the experimental work, this NIRT project also involves theory. As shown here, we have successfully simulated the 4x1 tetramer reconstruction using theoretical calculations by SIESTA, an algorithm for determining electronic and spatial structure of bulk materials and surfaces. The excellent agreement of the results of the calculations and simulations with the experimental observations gives great confidence for next steps of this project.

NIRT: Building Nanospintronic and Nanomagnetic Structures: Growth, Manipulation, and Characterization at the Atomic Scale

Arthur R. Smith, Saw-Wai Hla, Nancy Sandler, and Sergio E. Ulloa
Ohio University, Athens, OH, DMR-0304314
(work also partly supported by DMR-9983816).

OUTREACH

Formed an educational website with tutorial articles for students at a high school level, as well as research information. The articles were written by journalism undergraduate students **Sarah Laubacher** and **Anita Martin**.



http://nsnm.phy.ohiou.edu/index.php

NIRT: Building Nanospintronic and Nanomagnetic Structures: Growth, Manipulation, and Characterization at the Atomic Scale; Arthur R. Smith, Saw-Wai Hla, Nancy Sandler, and Sergio Ulloa, Ohio University, Athens, OH, DMR-0304314. The NIRT outreach efforts are gaining momentum as our new NSNM (Nanospintronics and Nanomagnetics) website is nearing official launch. Already the site is accessible through the given URL. Within the site are areas for students to find articles on nanoscience. One innovation is for the articles to function as tutorials, and since our NIRT topic is focused on spin, we call these "spintorials." It should be mentioned that we have already posted 2 "spintorial" sequences which were written by undergraduate journalism students at Ohio University last spring. We are also creating a glossary of terminology. Under "schedule visits," teachers and schools can also request visits of the NIRT PI's for the purpose of making presentations on nanoscience topics. As well, there is a location within the teaching and outreach section called "demos" for teachers to view presentation topics for K-12 visits. Currently, a flyer is being created by our new nanoscience journalism graduate student, which will be used to advertise our outreach program to area K-12 schools.